Simulation of Eu3+ luminescence spectra of borosilicate glasses by molecular dynamics calculations

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Résumé en anglais	Simplified inactive rare-earths doped nuclear waste glasses have been obtained by molecular dynamics (MD) simulation in order to investigate the local structure around the rare-earth by luminescence studies. MD calculations were performed with modified Born–Mayer–Huggins potentials and three body angular terms representing Coulomb and covalent interactions. Atomic positions within the glasses are then determined. Simulations of luminescence spectra were then obtained by calculation of the ligand field parameters affecting each luminescent ion. Considering the C2v symmetry, it is possible to calculate the radiative transition probabilities between the emitter level, 5D0, and the splitted receptor levels, 7FJ (J = 0–3) for each Eu3+ ion. The simulated emission spectra are obtained by convolution of all the Eu3+ ions contributions. A comparison with the experimental data issue from fluorescence line narrowing and microluminescence spectroscopies allowed us not only to validate the simulation of luminescence spectra from simulated environments, but also to confirm the presence and the identification of two major Eu3+ sites distribution in the nuclear glasses thanks to spectra-structure correlations.
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